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Reference materials — Guidance on, and keywords used for, RM categorization

Matériaux de référence — Conseils sur, et mots-clés pour, la catégorisation des matériaux de référence

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Foreword

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ISO/TR 10989 was prepared by the ISO Committee on reference materials (REMCO).

Introduction

Reference materials (RM) are a major tool for assuring quality and reliability of results obtained in analysis and testing. Laboratories active in these fields often face problems in identifying reference materials which suit their needs. Although a large number of producers of (certified) reference materials exist, presentation of the product spectrum of each of these producers is largely heterogeneous and follows quite different principles which, in particular, causes the above problem.

It was therefore considered necessary to conduct a study into existing schemes for RM categorization with a specific view to possible harmonization approaches.

This document reports on existing categorization schemes, describes the principles and the layout of a harmonized scheme, and contains a comprehensive list of keywords recommended for RM categorization.

Reference materials — Guidance on, and keywords used for, RM categorization

1 Scope

This Technical Report covers

a) the results of a study into, and comparison between, existing classification and categorization schemes for reference materials,

b) the development of reference material (RM) features and characteristics upon which a harmonized and consistent categorization scheme could be based, and

c) approaches for making the categorization scheme adaptive to new RM needs and developments.

The development of a harmonized categorization scheme aims at facilitating a transparent and comparable presentation of reference materials by producers, and the identification of reference materials by users. The intended categorization scheme was conceived to meet the needs of modern forms of information presentation and retrieval, i.e. internet-based catalogues and databases, and has been developed specifically with the view to being used this way.

2 Abbreviated terms

CCQM	Consultative Committee for Amount of Substance — Metrology in Chemistry
COMAR	International database for certified reference materials
CRM	Certified reference material
ERM®	European Reference Materials
ILAC	International Laboratory Accreditation Cooperation
IRMM	Institute for Reference Materials and Measurements
LGC	Laboratory of the Government Chemist
RM	Reference material
VIRM	Virtual Institute for Reference Materials

3 Existing categorization schemes

Eight major categorization schemes have been analysed, namely:

— the scheme as proposed by ILAC;

— the scheme applied and used by LGC Promochem (for presentation of RM in 5 field-specific catalogues: clinical, environmental, food, inorganic, physical);

— the COMAR scheme;

— the scheme provided by the VIRM database;

— the scheme used for presentation of the product spectrum by FLUKA Chemie AG;

— the IRMM scheme;

— the ERM® scheme;

— the scheme used by the CCQM for categorization of CMCs.

Most of these schemes use different perspectives on RM for categorization, and as a rule in a mixed (heterogeneous) form. In particular, this becomes obvious from the categorization scheme used by the VIRM initiative which uses “discipline” and a “generic term” as categorization criteria. The term list for “discipline” is not comprehensive, but homogeneous to a certain extent, while the term list for “generic” mixes up matrices and/or origins of (C)RM with properties and even uses and applications. Analyte and matrix are not categorized in the VIRM scheme. It should, however, be noted that VIRM uses more than one criterion for (C)RM description.

Main perspectives are the (certified, if applicable) reference property carried by the material, the field of application, and the analyte and/or matrix. The extent to which the different perspectives are mixed is different for different schemes, but a certain heterogeneity is always present. LGC Promochem simply sub-divides the whole set of available RM and assigns the sub-groups to five different catalogues with the aim to assure that the within-catalogue categorization scheme does not become too heterogeneous and matches terminologies established within the different fields of application. Although the CCQM scheme is the most homogeneous of all schemes considered, the degree of detailing is not very high. A scheme designed to facilitate the identification of reference materials by users should therefore be designed by integration of the various reasonable approaches of the above (and other, if available) schemes.

For pharmaceuticals, the USP model for drug characterization was investigated with a clear view to therapeutical categorization which is mainly governed by defining (groups of) active agents with specific potency and, consequently, specific uses and applications.

4 The harmonized scheme

4.1 Basic principles

Given the results of the above preliminary study, the following basic ideas can be developed for a harmonized categorization scheme.

Depending on the intended purpose of a reference material, the valuable property (i.e. the one a customer pays for and which normally also distinguishes this specific material from the rest) may be of different kinds. There are RM carrying an obviously material-dependent property, however the material itself is of minor or no interest to the user since the user is interested only in this specific property. This is the reason why “single” categorization schemes are normally heterogeneous.

EXAMPLE 1 An oil may be produced to carry a certain value of viscosity, and customers will not (or at least only to a minor extent) be interested in knowing whether the oil is mineral or synthetic. On the other hand, for a transformer oil developed for residue analysis (e.g. PCBs), viscosity may be of minor or no interest to the user since the analytical method of choice normally includes a matrix separation.

Heterogeneous categorization schemes often create problems in assigning the appropriate category to a specific material, especially when more than one apply. On the other hand, the degree of detailed description may be extremely different for the different categories of the scheme.

EXAMPLE 2 Compare a group named “low alloy steels” with a group called “life science applications”. The latter is clearly in disadvantage.

It cannot be the intention of the categorization scheme to assign a unique keyword sequence to each and every RM, existing or intended to be produced. This makes such a scheme different from e.g. the unique identification of a substance by a CAS number. The only intention is to provide a descriptive tool allowing the creation of sufficiently large (for representativeness) and sufficiently fine-tuned groups of resembling RM. Group sizes may significantly vary from group to group depending on the total number of RM available on the market for the specific purpose, and the (economic and scientific) importance of this share.

Given this, an ideal categorization scheme should be

a) “as distinctive as possible” (i.e. a possibly more detailed description for distinction), and

b) “as appropriate as necessary” (i.e. good enough for separating between different purposes/uses, but not unique).

These goals cannot be achieved within the framework of one single, stiff categorization scheme even if one allows the scheme to be (extremely) heterogeneous.

4.2 Layout

Reference materials should therefore be categorized in a more descriptive, flexible approach. This approach describes the material according to the three criteria identified earlier, namely

(certified) reference property — (field of) application — analyte and matrix.

For each of the three criteria, lists of keywords (i.e. groups and subgroups) are given in Annex A. Criteria/descriptions of a specific RM (consider the oil carrying a value for viscosity) which do not apply may be left out in the description. This should appropriately be indicated in the presentation.

The keywords of the categorization schemes used or proposed by ILAC, LGC Promochem (five catalogues), COMAR, FLUKA, IRMM, ERM®, and the CCQM (as studied under Clause 3) have been split off according to the three criteria (or perspectives) to look at an RM. From the collation of keywords from all schemes, the list as presented in Annex A was generated. This “symbiosis” list was created with the intention of either including a specific keyword from a particular categorization scheme or making sure that a coarse category (e.g. “high-purity chemicals”) could be described by a combination of criteria from the symbiosis list.

Reference materials carrying two or more different reference properties cannot be described by a single category sequence.

EXAMPLE A silicon nitride certified for trace element content and phase composition.

In such situations, several keyword sequences (according to the number of reference properties carried by the material) can be attributed. From the point of view of information retrieval, this will ensure that the material can be found and compared with competitive materials for all purposes/uses for which it is intended.

4.3 Recommendations

The keywords as listed in Annex A are intended for structuring, in a harmonized way, the presentation of any particular set of reference materials offered to the customer. They may be applied to any presentation form, but apply mainly to databases and catalogues, both electronic and printed. The keyword list of Annex A is not exhaustive, in particular with a view to new categories emerging on the basis of scientific and technical progress.

It must also be pointed out that the scheme as proposed in Annex A does not affect the producer's internal scheme of attributing serial or otherwise structured numbers to particular materials. It is for external presentation, search and retrieval purposes only.

The scheme could be understood as an offer made to RM producers. Depending on the intention of the producer and the kind of material, producers may select the degree of detail they implement in the keyword sequence. Certainly the recommendation for an “as good as possible” description using the available category

keywords can be given, but it is up to the producer to decide whether or not a particular keyword applies and should be included in the presentation.

Producers should therefore decide about the number of criteria they wish to apply for structuring their production profile presentations. It is in no way mandatory to use all ordering criteria. In principle, any set of reference materials should be categorized

a) with a satisfactory degree of distinction between the different materials, but

b) without the intention to make all categories unambiguous.

The above principle equally applies to the number of criteria used, and the keyword sub-level attributed to a particular reference material.

EXAMPLE Depending on the position of a particular producer of food reference material in the market, it may be sufficient to use the category “beverages” if it is known that the producer specializes in, for example, non-alcoholic beverages. If this is not the case, a lower sub-level (e.g. “alcoholic and low alcohol beverages”) can be chosen in order to distinguish these products from others.

It is, however, not recommended to mix up categories originating from, and belonging to, different aspects/ criteria of categorization.

5 Reporting attributed keywords

For electronic search and data retrieval, catalogue search using the descriptive keywords in the three categories as given is recommended. Producers and distributors of reference materials operating data retrieval systems which are publicly accessible and/or provide product lists or catalogues should analyse the ways (i.e. perspectives) used by customers to seek information on the availability of a specific reference material meeting customers' needs. Experience shows that almost all three main perspectives (certified property, field of application, and analyte/matrix combination) are used by customers potentially interested in reference materials.

Providers of electronic or written data collections on reference materials (producers, distributors, consultants, etc.) should therefore:

a) categorize each material available as fully as possible according to the keywords given in Annex A;

b) indicate, for each material, the above defined descriptive keywords in an appropriate form (possible forms are, for example, sub-headers on printed material specifications and/or in printed catalogues, and specific search fields in electronic data collections);

c) provide search tools for the above defined keywords (catalogue search).

It is not always feasible, in some cases even senseless, to attribute keywords for all three main perspectives/criteria to any particular reference material. Reference materials for, for example, dimensional properties do not contain “analytes”, and the material they are made of is normally of minor importance (at least for the user). In those cases, the corresponding categorization field should be left blank or filled in with “n/a” (see also Clause 4).

Thus, a complete categorization may look like:

```
reference property:     nutritional properties
application:            food analysis
analyte:                ethanol and alcohol congeners
matrix:                 alcoholic and low alcohol beverages
```

It describes the property as nutritional, the field of application as food analysis, the analyte as ethanol and alcohol congeners, and the matrix as alcoholic and low alcohol beverages. There may be doubts whether an

alcoholic content is actually a “nutritional” property. To be on the safe side, the first descriptor could be replaced by “food properties”.

6 Category keyword coding

Providers of electronic or written data collections on reference materials might wish to convert the keyword sequences attributed to reference materials into a machine-readable code. Appropriate coding schemes for the generation of a compact descriptive identifier which can be used for all information retrieval purposes may be developed in different ways. A simple coding scheme could be based upon the following principles.

— Three digits for each of the criteria “Reference value” and “Application” are reserved, although not all of them may be occupied, depending on the sub-group level used for categorization.

— “Analyte” and “Matrix” are described by four digits each, combined giving an (up to) 8-digit code for this criterion. The first digit for each criterion is alpha-numeric, the others are numbers.

Codes generated from these rules are not descriptive for the key word although there are some correlations, especially for the matrix criterion. As a code for “not applicable”, a numerical zero may be used in the first digit of the corresponding criterion, distinguishing it clearly from the letters in case the criterion is applicable.

NOTE It should be pointed out that this “machine-readable” code generated for electronic search and retrieval purposes is not intended to be printed in the documentation accompanying the reference material, as e.g. passport, certificate, label or other (although this option is not excluded).

The following examples of how the descriptors of the proposed scheme could be applied are taken from different CRM producers and refer to different materials with different fields of application.

EXAMPLE 1 Material: ERM BA005 Lager 5 % ABV (alcohol by volume) (5,07 ± 0,03 % ABV). According to Clause 5, the complete categorization would be:

```
reference property:   nutritional properties
application:          food analysis
analyte:              ethanol and alcohol congeners
matrix:               alcoholic and low alcohol beverages
```

EXAMPLE 2 Material: NIST SRM 3145a – Rubidium Standard Solution. The categorization would be:

```
reference property:   trace component content
application:          single element standards for ICP
analyte:              alkali metals
matrix:               solvents
```

Annex A
(informative)

List of keywords for RM categorization

A.1 Keywords according to criterion I: (certified) reference property

Main group	Sub-group 1st level	Sub-group 2nd level
biological properties	biological activity genetically modified organism (GMO) content enzyme activity protein interaction	
cell properties	object number multiplication/decay rate	
chemical composition	blanks extractable element content isotope abundance ratio major components mixtures purity stoichiometry species content trace component content	
chemical properties	atomic weight molecular weight catalytic activity chain length identity polarity sequence	
fire resistance properties	flammability smoke density	
food properties	blanks fatty acid profile nutritional properties proximates sensory properties triglyceride composition	
moisture		

Main group	Sub-group 1st level	Sub-group 2nd level
physical properties	age	
	dimensional	length volume roundness step height
	electrical	conductivity dielectric strength resistivity
	magnetic	magnetic susceptibility
	mechanical	
	optical	colour density optical rotation refractive index reflectance spectral absorbance spectral emission spectral parameters
	physicochemical properties	density electrolytic conductivity electrophoretic mobility pH surface tension viscosity
	radioactivity	
	structural properties	crystallographic structure morphological properties phase composition single crystal cell parameters
	thermodynamic properties	boiling point Curie point enthalpy and heat capacity flash point melting, freezing and triple points temperature fixed point thermal conductivity thermal expansion thermal resistance vapour pressure

Main group	Sub-group 1st level	Sub-group 2nd level
technical properties	abrasive wear rate scratch resistance corrosion rate creep rate creep rupture time elasticity fatigue rupture life hardness impact toughness fracture toughness tensile strength	
humidity		
properties of films and surfaces	depth profiling ion beam sputtering nominal thickness particle backscattering x-ray fluorescence surface finish surface roughness	
sizing	particle number particle distribution particle flow particle size porosity surface area	
miscellaneous		

A.2 Keywords according to criterion II: (field of) application

Main group	Sub-group 1st level	Sub-group 2nd level
age determination		
buffer systems		
calibration	electrode calibration spectrochemical materials spectrochemical solutions	 single element solutions for ICP single element solutions for AAS multi-element solutions for ICP multi-element solutions for AAS
cell biology		
clinical/medical applications	bacteriology and mycology clinical chemistry laboratory medicine haematology and cytology immunology molecular biology parasitology tissue pathology virology other clinical/medical	 DNA profiling DNA sequencing
cosmetic industry		
electrophoresis		
elemental analysis		
environmental analysis		
fluorescence analysis		
food analysis		
geochemical analysis		
geophysical analysis		
metal analysis		
radiation dosimetry		
speciation		
thermal analysis		
fire research		

Main group	Sub-group 1st level	Sub-group 2nd level
forensic applications		
identity and authenticity test	fibre identification substance identification	
internal quality control		
method-specific applications	chromatography dosimetry microscopy spectroscopy titration x-ray diffraction	GC ion chromatography LC thin-layer chromatography
non-destructive testing	dye penetration magnetic particle inspection	
pharmacopoeial standards		
miscellaneous		

A.3 Keywords according to criterion IIIa: analyte description

Main group	Sub-group 1st level	Sub-group 2nd level
chemical elements	alkali metals alkaline earth metals halogens metalloids noble gases non-metals other metals rare earth metals transition metals	
electrolytes		
ethanol and alcohol congeners		
ions	anions cations	
isotopes	natural isotopes induced isotopes radioactive isotopes radiogenic isotopes stable isotopes isotopically labelled compounds	

Main group	Sub-group 1st level	Sub-group 2nd level
metal-containing compounds	minerals	
	metallo-organic compounds	
organic compounds	additives	acidity regulators
		antioxidants
		colouring agents
		emulsifiers
		fillers
		plasticizers
		vulcanising agents
		other
	amino acids	
	carbohydrates	
	chiral compounds	
	copolymers	
	creatinine	
	DNA and RNA	
	drugs of abuse	
	enzymes	
	erythrocyte protoporphyrine	
	ethylglucuronide	
	hormones	
	lipids	
	mycotoxins	
	peptides	
	pesticides	acaricides
		fungicides
		herbicides
		insecticides
	polymers	
	priority pollutants	AOX
		BTEX
		heavy metals and metal species
		organo tin compounds
		PAH
		polyhalogenated compounds
		TPH
	proteins	
	steroids	
	toxins	animal origin
		plant origin
		other biological origin

Main group	Sub-group 1st level	Sub-group 2nd level
	therapeutic drugs	analgesics anesthetics antibacterials anticonvulsants antidementia agents antidepressants antidotes, deterrents, and toxicologic agents antiemetics antifungals antigout agents anti-inflammatories antimigraine agents antimyasthenic agents antimycobacterials antineoplastics antiparasitics antiparkinson agents antipsychotics antivirals anxiolytics bipolar agents blood glucose regulators blood products blood modifiers blood volume expanders cardiovascular agents central nervous system agents dental and oral agents dermatological agents enzyme replacements/modifiers gastrointestinal agents genitourinary agents hormonal agents, stimulant/replacement/ modifying hormonal agents, and suppressant immunological agents inflammatory bowel disease agents ophthalmic agents otic agents respiratory tract agents sedatives/hypnotics skeletal muscle relaxants therapeutic nutrients/minerals/ electrolytes
	veterinary drugs vitamins VOC	
respirable silica		
radiopharmaceuticals		
miscellaneous		

A.4 Keywords according to criterion IIIb: matrix description

Main group	Sub-group 1st level	Sub-group 2nd level
acids and bases	pure acids and bases industrial acids and bases	
agricultural chemicals and fertilizers animal body fluids animal tissues ashes and dusts biological reference cultures bio-stabilization products carbides catalysts cements, clays and related products ceramics, glasses and refractory oxides dyes explosives, primers, degradation products flammable liquids and residues thereof		
food	additives dyes preservatives and antioxidants spices	
	beverages	alcoholic and low alcohol beverages non-alcoholic beverages
	fruits vegetables cereals dairy products	
	fats	animal oils and fats vegetable oils and fats
	fish	sea and freshwater fish molluscs plankton
	meat processed food	
fibres	asbestos fibres natural fibres synthetic fibres	
filters and filter media		

Main group	Sub-group 1st level	Sub-group 2nd level
fuels	biofuels	
	gaseous fuels	
	liquid fuels	
	solid fuels	coal and coke
		wood-based fuels
gases	balance gas	air
		synthetic air
		nitrogen
		oxygen
		noble gases
	multiple-component mixtures	natural gas
		emission gases
genetically modified objects		
industrial glasses	automotive	
	bottle	
	spectacle	
	window	
human body fluids	blood	
	plasma	
	serum	
	saliva	
	urine	
human body tissues	bone	
	hair	
	skin	
	organs	
metals	cast irons	
	high purity metals	
	ferrous metals	
	non-ferrous metals and alloys	Al, Mg, Si and alloys
		Li, Be, alkali and alkaline earth metals
		Cu, Zn, Pb, Sn, Bi and alloys
		Ni, Co, Cr and alloys
		Ti, V, Zr and alloys
	precious metals and alloys	
	rare earth metals	
	refractory metals and alloys	
	steels	raw material
		high alloy steels
		low alloy steels
		special alloys
		unalloyed steels
minerals		

Main group	Sub-group 1st level	Sub-group 2nd level
mineral processing materials	furnace matte converter matte concentrate mill feed tails	
noxious substances		
ores and rocks		
oxides and salts		
petroleum products	heat exchange fluids oils and lubricants	
paints and varnishes	architectural automotive	
particulate materials		
plastics and rubbers		
plants	aquatic plants grasses and crops trees and bushes other	
polymers		
sediments	freshwater sediments marine sediments	
semiconductors		
sludges		
soils		
solvents		
wood	wood products	
waste		
water	potable water fresh water sea water waste water sewage	
miscellaneous		

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